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DESIGN OF A FLOW FACILITY FOR QUANTITATIVE SPECTROSCOPIC STUDIES OF HIGH TEMPERATURE SPECIES

by

Michael E. Gersh and Charles E. Kolb

Prepared Under
Contract No. F49620-77-C-0075

April 1978

Prepared for

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
Building 410
Bolling AFB, D.C. 20332

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ABSTRACT

The objective of this study is the measurement of the infrared absorption coefficients and absorption line spacing of several boron compounds in the gas phase over the temperature range of 300 to 1500°K. In the past year, the following technical progress was made. The apparatus was designed, and the variable temperature flow tube in which the boron compounds are made by reaction was constructed. In initial tests the flow reactor achieved its design temperature of 1500°K, while using only half of the available power of the heating elements. In addition, a separate flow simulation experiment in a scale model of the flow tube was used to verify the design of the critical spectroscopic analysis region and to establish the range of flow conditions over which the flow will be well behaved. Finally, the optical system for the low resolution spectroscopic measurements was fabricated and assembled on the apparatus.

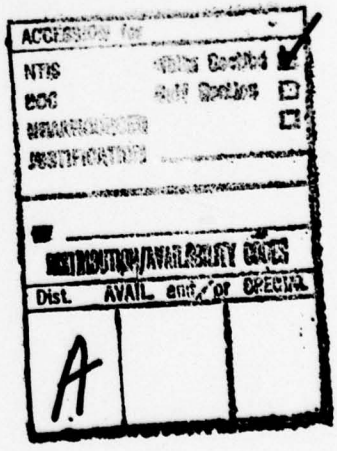

TABLE OF CONTENTS

1. INTRODUCTION

The objective of the present research program is the performance of quantitative spectroscopic measurements on a number of boron oxides, fluorides, and oxy-fluorides. The measurement program is designed to produce results which are suitable for use in infrared radiation band models[1], and, therefore, the infrared absorption measurements will be performed at high spectral resolution, as well as at low spectral resolution. This will permit the determination of the two band model parameters the average absorption coefficient and the fine structure parameter[1]. In addition, the measurements will be performed within the temperature range of 300-1500°K, with a possible extension to 1800°K. At present, it is anticipated that measurements will be performed on the species BF_3, BF, OBF, HBO_2, and BO_2. These species must be produced in high temperature reactions, with the exception of BF_3 which is a commercially available gas.

A conceptual diagram of the experimental apparatus is shown in Figure 1. The species of interest are produced by reaction in, or introduced into, a variable temperature flow reactor. Then, the flow is passed through an analysis region in which a multi-pass absorption cell (White cell) [2] is mounted perpendicular to the flow direction. Finally, a portion of the flow is sampled by a molecular beam mass spectrometer before being exhausted to a large mechanical vacuum pump. Since the number density of the absorbing species is measured in-situ by the mass spectrometer, one can obtain absolute values for the absorption coefficients without assuming that the reactive species in the flow tube have achieved local thermodynamic equilibrium.

The remainder of this report is organized as follows: The details of the apparatus will be described in Section 2. A flow simulation study that was undertaken in support of the design of the crucial analysis region will be described in Section 3.

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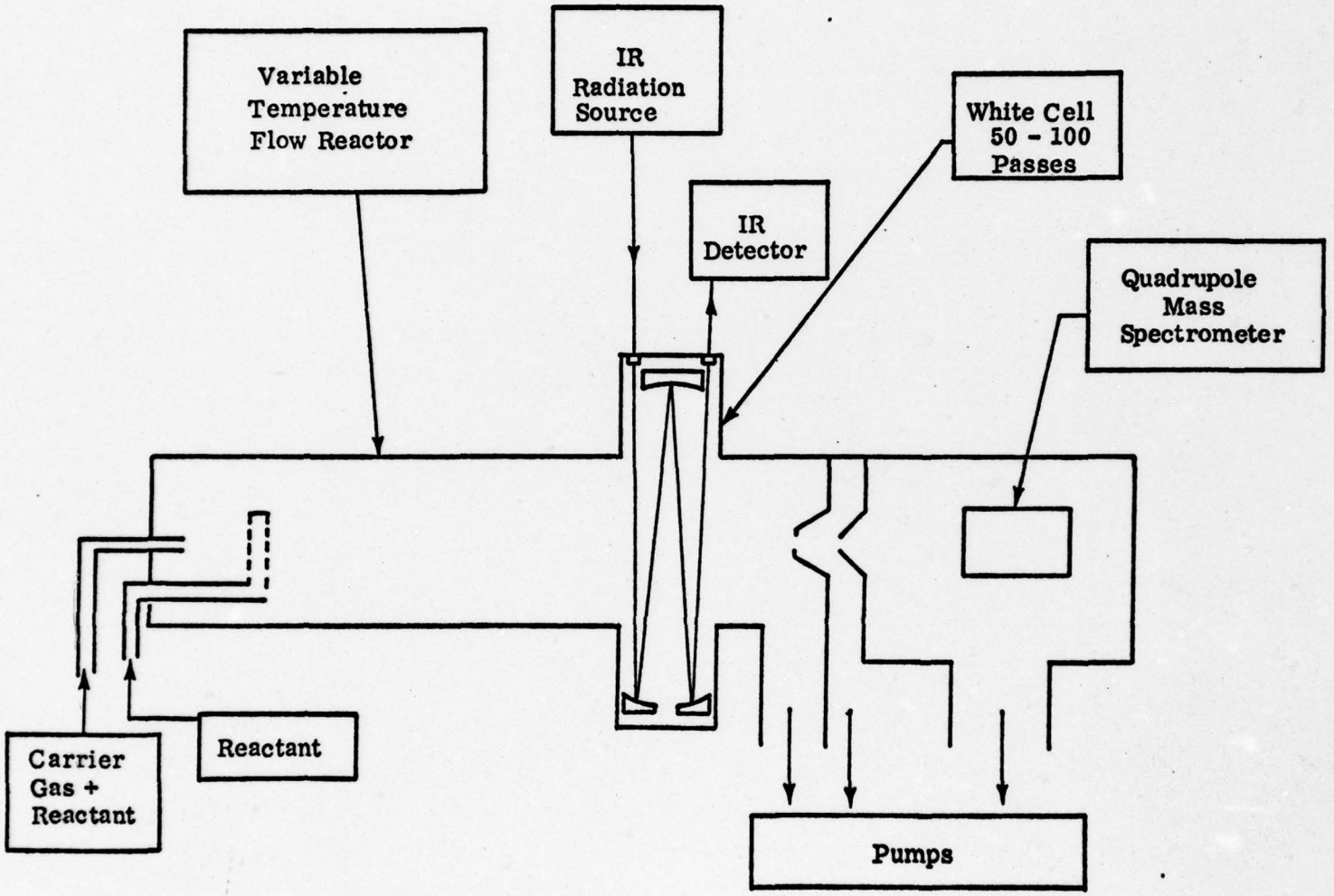

Figure 1. Conceptual Diagram of Flow Reactor/Infrared Spectrometer

Finally, the present status of the contractual effort will be summarized in Section 4, along with a brief discussion of the plans for work in the immediate future.

2. APPARATUS DESCRIPTION

The design of the variable temperature flow reactor is shown in Figure 2. The outer vacuum jacket is constructed of steel and is water-cooled, as are the aluminum end plate assemblies. The water cooling protects temperature-sensitive components and ensures stability of the White Cell dimensions. The "rear" end plate holds the alumina flow tube, as well as power gas and thermocouple feedthroughs. The "front" flange is designed for mounting to the quadrupole mass spectrometer or to a blank flange for tests and for experiments for which mass spectrometer sampling is not required. In the analysis region, eight four-inch flanges are placed around the circumference of the vacuum jacket. Four of these ports are connected by alumina tubes to the main flow tube and provide for optical analysis of the hot flowing gas. This optical analysis can consist of absorption or emission measurements using the White Cell or of fluorescence measurements using two ports at right angles to each other. One of the remaining four ports is presently connected to a Kinney Vacuum KMBD 1602 mechanical vacuum pump with an effective pumping speed of approximately 1000 cfm. The other three ports are presently unused.

The main elements of the thermal design include the heating elements and the surrounding layer of refractory insulation. The refractory insulation is composed of a self-supporting "spool" of rigid alumina fiber insulation (Zircar Products, Inc.), upon which is wound several layers of Zircar alumina fiber blanket insulation, followed by additional layers of Carborundum Company alumina-silica blanket insulation. The insulation assembly has an inside diameter of 6 inches (15 cm) and is designed to withstand continuous operating temperatures in excess of 1800^{o}K. The commercially-available Kanthal A-1 heating elements that are currently being used have a design temperature rating of 1500^{o}K and a power capability of over 6 kW (Thermcraft, Inc. type RH). The heaters are supplied with power by Love Controls Corporation solid-state temperature

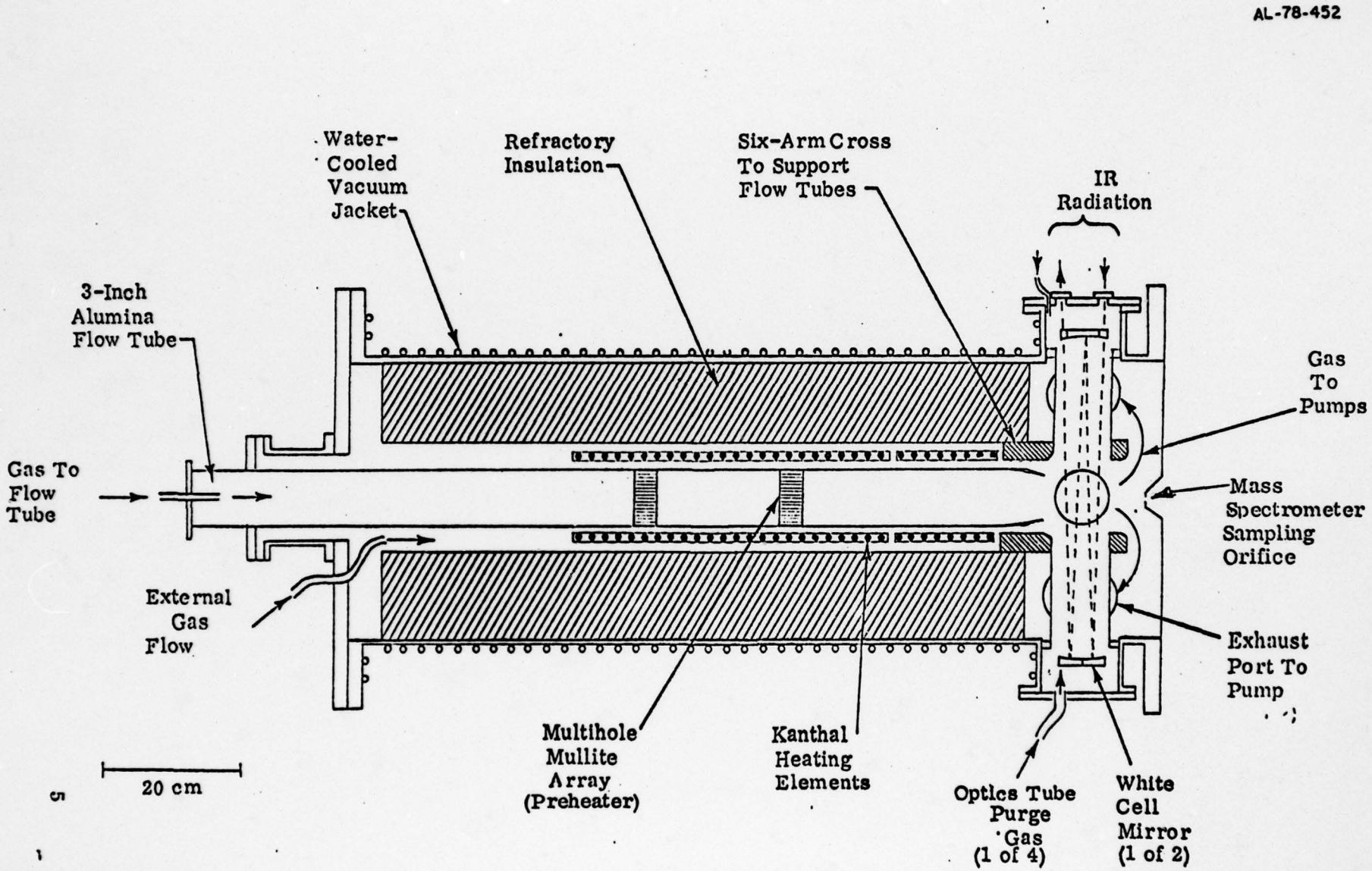

Figure 2. Cross Sectional View Of Heated Flow Reactor

controllers and power supply units. In preliminary tests, the fully assembled flow reactor achieved a temperature of 1500°K with a power consumption of less than 3 kW. Thus, the thermal design of the flow reactor is adequate for the performance of experiments at 1500°K. Finally, it should be noted that the flow reactor could be operated at a temperature of 1800°K if one replaced the Kanthal heating elements with platinum-rhodium heater wire wound around the central alumina flow tube. This would also require a small change in the power supply circuit.

The design of the gas flow system within the variable temperature flow reactor is fairly complicated due to the constraints imposed by the necessity of making infrared absorption measurements in the analysis region. Figure 2 shows the configuration that will be used in the initial measurements on BF_3. The main flow inside the 2 7/8 inch (7.3 cm) inside diameter 99.8% alumina flow tube (McDanel Refractory Porcelain Company) contains argon carrier gas + BF_3. This gas is heated as it passes through two preheaters which are 1 inch (2.5 cm) thick mullite ''honeycomb'' hole arrays having 1.6 mm (1/16 inches) round holes and a 67% frontal open area (General Refractories Company). The heated gas then passes through an isothermal region of the flow tube and a subsonic nozzle before entering the spectroscopic analysis region. A second, external flow of Ar passes around the outside of the main flow tube and through a coaxial, annular subsonic nozzle, after which it merges with the main, core flow. In addition, small flows of Ar are added to each of the four optics tubes as a purge gas in order to keep the optics clean. The six flows of gas meet in the center of the analysis region in a section of the flow system that is made from Cotronics Corporation 960 machinable alumina ceramic. This six-arm cross piece supports the main flow tube and the four optics tubes. However, its main purpose is to provide an environment in which the flow from the main tube will be well-behaved as it traverses the White Cell, impinges on the mass spectrometer sampling orifice, and is exhausted by the mechanical pump. Thus, the design of this element of the flow system is particularly important to the success of the experimental

program, and a separate experimental study was undertaken in order to ensure that the proposed design would adequately control the gas flow in the analysis region. This study is described in Section 3 of this report.

The design of the present external optical system for the infrared absorption measurements is shown in Figure 3. This double beam optical system has been designed for the initial, low spectral resolution measurements. The infrared radiation source is a Perkin-Elmer Corporation "Opperman Source" which is used in their current infrared spectrometers. The radiation impinges on a mirror-bladed, 50% duty cycle chopping wheel (Valtec Corporation) which alternately allows it to pass into the White Cell or reflects it, thereby bypassing the White Cell. In Figure 3, M2, M3, M4, M7, and M8 are flat mirrors: M1 and M9 are spherical mirrors; and M5 and M6 are off-axis paraboloid mirrors. The beam splitter is made of uncoated zinc selenide, the monochromator is a Spex Minimate, and the detector is a Santa Barbara Research Corporation HgCdTe photoconductive detector, in front of which is placed an order-sorting (long wavelength pass) filter in order to avoid interference from higher order diffraction in the monochromator. Since the optical system consists of reflective optics (except for the zinc selenide beam splitter), it is achromatic, and it can be aligned with the use of a helium-neon laser.

The only other major subsystem that must be completed is the interface between the variable temperature flow tube and the molecular beam mass spectrometer. This will be accomplished in the second year of the contract.

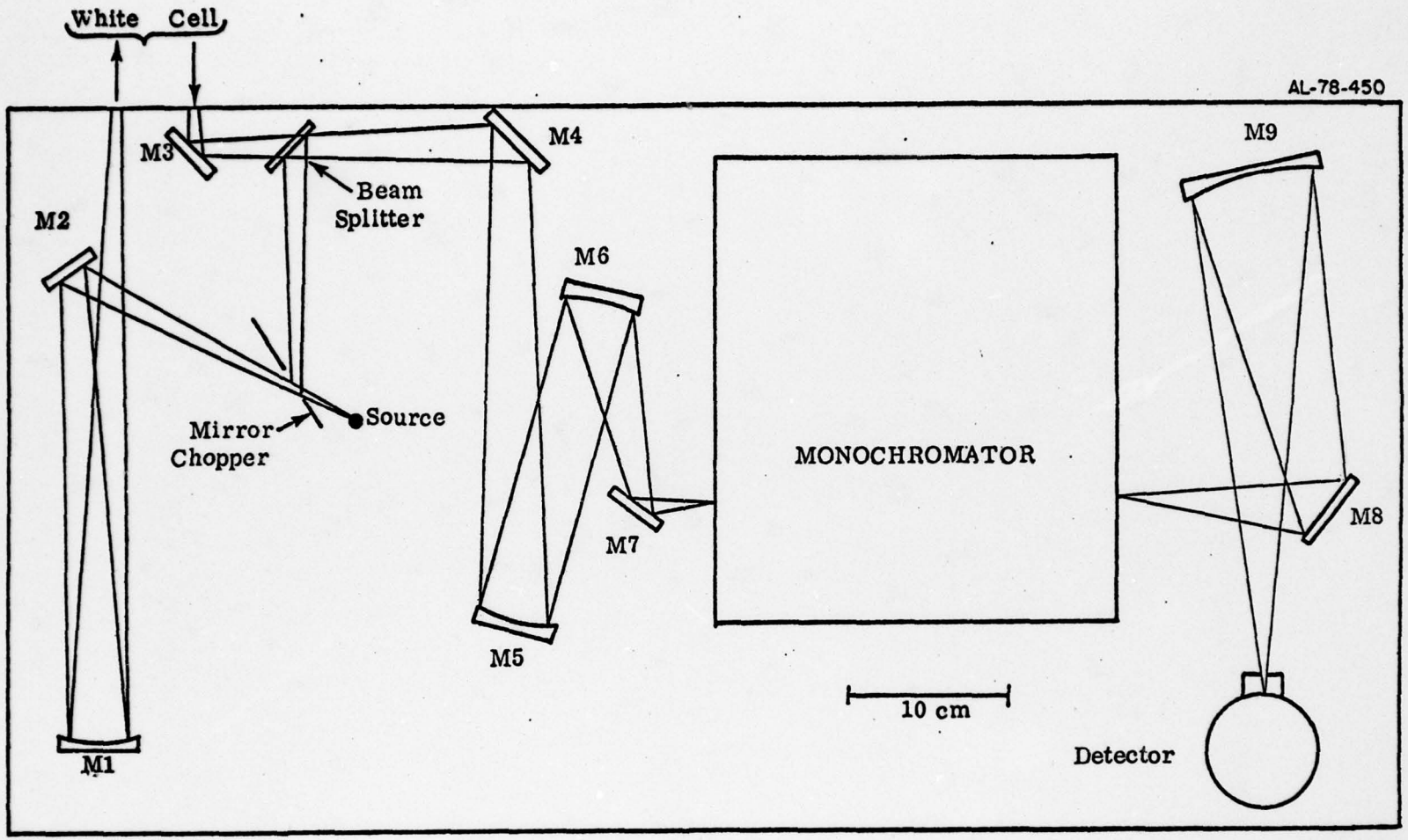

Figure 3. View of External Optics

3. FLOW SIMULATION STUDY FOR ANALYSIS REGION

As was noted in Section 2, a crucial element of the apparatus design is the configuration of the flow system in the spectroscopic analysis region of the variable temperature flow tube. In order for one to be able to perform quantitative absorption (or emission) measurements on the flow tube gases, three criteria must be satisfied: (1) the geometry of the absorbing gas flow must be well defined in the region where it traverses the White Cell; (2) the flow in this region must be stable; and (3) the temperature of the absorbing gas flow must be well defined (and, preferably, the gas should be isothermal). To satisfy these criteria, the absorbing flow should ideally be confined in a cylindrical geometry and be located in a stable position, without any recirculation of absorbing gas into the optics tubes (i. e., the flow should behave as if it were confined by a cylindrical tube). For an ambient temperature flow tube with single-pass optics, one could simply place optical windows on the flow tube; however, the present experiment requires high absorbing gas temperatures and a multi-pass absorption cell (for additional sensitivity). This necessitates the use of a wall-less confinement of the absorbing gases as they pass through the analysis region. This can only be accomplished by fluid mechanical confinement of the absorbing gas flow.

The analysis region design shown in Figure 4 was considered to be most promising. Here, the main, absorbing gas flow and the outer, coaxial "shield" gas flow are both passed through subsonic nozzles, after which they join and pass through the analysis region. The area ratio of the main flow nozzle to the shield flow nozzle is 2:1, and the corresponding flow rates are also designed to be in a 2:1 ratio so that the velocities of the two flows will be the same when they meet downstream of the nozzles. In addition, it was estimated that the flow of purge gas into the optics tubes should equal approximately 10% of the main flow and should be evenly divided between the four optics tubes.

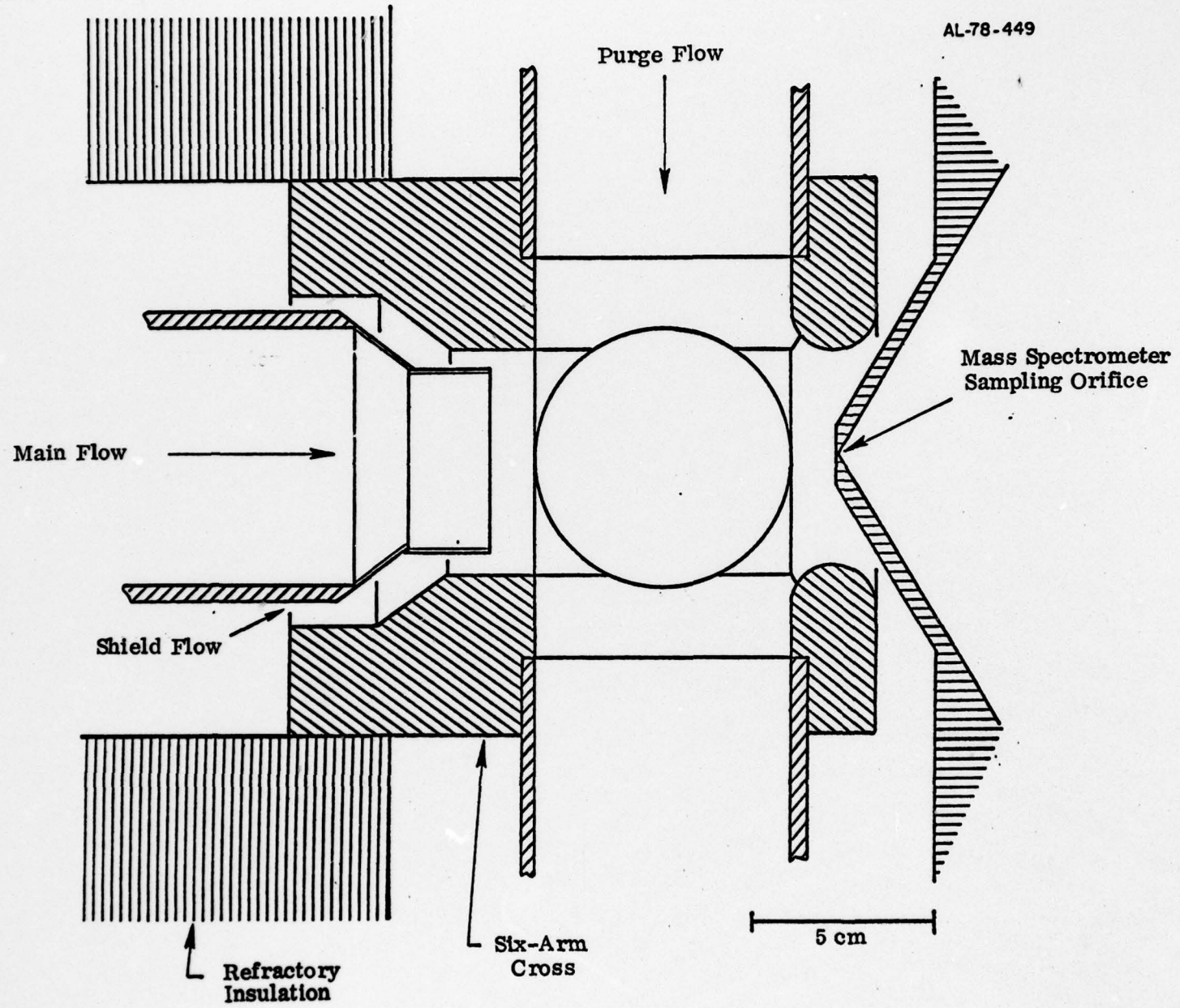

Figure 4. Cross Sectional View of Analysis Region

This flow geometry is considerably more complicated than that used previously for flow reactors[3, 4], and the design criteria for the confinement of the absorbing gas flow are quite strict. Thus, it was concluded that this crucial element of the flow system design should be tested in a flow simulation experiment before the fabrication of the six-arm cross out of machinable alumina ceramic. This would obviate the need for a major system redesign if the initial design proved to be inadequate and would establish the approximate range of operating flow conditions over which the flow confinement of the absorbing gas would be effective.

The flow simulation experiment was set up in the following manner: A 1/2 scale model of the flow system was fabricated out of plastic (polymethyl methacrylate) with flowmeters monitoring the main flow, the shield flow, and the four purge flows. The gas flow was simulated by using a water flow with the same Reynolds number, which is a standard technique in fluid mechanics and is valid for subsonic, incompressible flows[5]. The flow pattern is determined by injection of Fluorescein dye into any one of the water flows and observation of the bright halogen lamp.

The required water flow velocity (and, therefore, flow rate) is obtained from the flow velocity of Ar that is to be simulated by equating the Reynolds numbers of the flows:

$$\mathrm{Re} = \frac{\rho u d}{\eta} = \frac{\rho' u' d'}{\eta} \quad , \tag{1}$$

where ρ is the density, u is the flow velocity, d is the tube diameter, η is the viscosity, and the prime refers to the conditions for water. Then, we let $d' = 1/2d$ and $\rho = \rho_o P$, where $\rho_o = 2.35 \times 10^{-6}$ g/cm^3/torr and P is the Ar pressure in torr. Also, $\rho' = 1$ g/cm^3, $\eta = 2.2 \times 10^{-4}$ poise, and $\eta' = 1.0 \times 10^{-2}$ poise (at 20°C). This leads to the expression

$$u' = 2.1 \times 10^{-4} \text{ Pu.} \qquad (2)$$

Thus, for a given flow velocity u of Ar at 20°C and at a pressure P, we are able to obtain the water velocity u' that is required for the simulation. Of course, if one wanted to simulate Ar flows at other temperatures, one would then have to substitute the appropriate values of ρ and η.

When the flow simulation experiments were performed, a number of interesting results were observed. The major result is that with a Reynolds number for the main flow that is greater than approximately 100, and for the flow rate ratios given above (main: shield: purge = 10:5:1), the main flow appears to be stable and cylindrical in form as it passes through the analysis region. (From a practical point of view, it would be probably be wise to operate the flow reactor at Re $\gtrsim$ 200.) Under these stable flow conditions, no recirculation pattern of main flow water was observed in the "optics tubes". However, when dye was added to the water of the shield flow, a strong recirculation pattern of shield flow water was observed in the optics tubes, and this phenomenon persisted even at the highest main flow Reynolds number (560) used in the experiments. Thus, it may be concluded that a simpler flow configuration without a shield flow would not satisfy the analysis region design criteria since there would be recirculation of absorbing gas in the optics tubes. The present design is successful because only the non-absorbing shield gas recirculates in the optics tubes, while the main flow of absorbing gas is confined by the shield flow to a cylindrical region in the center of the analysis region. In addition, since the shield gas is at the same temperature as the main flow, the column of absorbing gas should be essentially isothermal.

Finally, it is interesting to examine the practical consequences of the flow limits of the present apparatus. If we assume a minimum Reynolds number of 200 and a carrier gas of room temperature Ar, we obtain the minimum flow velocity u at a pressure P from Equation (1). This yields

$$[uP]_{min} = 2560 \text{ cm/sec - torr.} \quad (3)$$

For example, the minimum room temperature Ar flow velocity at 10 torr would be approximately 2.6 m/sec. Conversely, the maximum flow velocity (within the limitations imposed by the pumping system) is determined by the Reynolds number above which the flow becomes turbulent. Since the transition region from laminar to turbulent flow occurs at Reynolds number of between 2, 000 and 10, 000[6], we may choose a value of 2, 000 as a safe upper limit. This yields the relation

$$[uP]_{max} = 25,600 \text{ cm/sec - torr.} \quad (4)$$

Thus, it should be possible to operate the variable temperature flow reactor over its projected operating range of 1-100 torr and 1-70 m/sec flow velocity (limited by speed of pump). If necessitated by the experiments, these operating ranges could be extended, subject to the constraints of Equations (3) and (4).

4. SUMMARY

The present status of the contractual effort may be summarized as follows: The apparatus has been designed, and the construction is largely complete. The major remaining construction job is the interface of the variable temperature flow reactor and the molecular beam mass spectrometer.

The initial low spectral resolution measurements will be performed on BF_3, since it is a commercially available gas. However, in-situ calibrations and checks of the apparatus will be performed with the use of CO as the absorbing gas since it has been studied much more extensively than BF_3, particularly at high temperatures. Subsequently, the spectral absorption coefficients of BF, BO_2, OBF, and HBO_2 will be measured at low spectral resolution. The major experimental challenge with these molecules will be the development of sources for the creation of these molecules by reaction in the flow tube or for the introduction of these molecules into the flow tube. Once the sources have been developed, the absorption measurements would be made in a relatively straightforward manner, following the procedures developed for BF_3.

Finally, longer range plans call for high spectral resolution measurements on the above species, which would be performed with the use of a tunable diode laser as the radiation source.

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REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER: AFOSR-TR-78-0966	2. GOVT ACCESSION NO. / 3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle): DESIGN OF A FLOW FACILITY FOR QUANTITATIVE SPECTROSCOPIC STUDIES OF HIGH TEMPERATURE SPECIES.	5. TYPE OF REPORT & PERIOD COVERED: Interim rept. / 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s): Michael E. Gersh, Charles E. Kolb	8. CONTRACT OR GRANT NUMBER(s): F49620-77-C-0075 new
9. PERFORMING ORGANIZATION NAME AND ADDRESS: Aerodyne Research, Inc., Bedford Research Park, Crosby Dr., Bedford, MA 01730	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: 61102F, 2303/B1, B1
11. CONTROLLING OFFICE NAME AND ADDRESS: Air Force Office of Scientific Research/NC, Bolling AFB DC 20332	12. REPORT DATE: Apr 1978 / 13. NUMBER OF PAGES: 18
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office): 24p.	15. SECURITY CLASS. (of this report): UNCLASSIFIED / 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

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17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Infrared
Spectroscopy
Boron Compounds
High Temperature

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

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20. ABSTRACT (Continued)

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